

Charmless chiral perturbation theory for $N_f = 2 + 1 + 1$ twisted mass lattice QCD

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Abstract

The chiral Lagrangian describing the low-energy behavior of $N_f = 2 + 1 + 1$ twisted mass lattice QCD is constructed through $O(a^2)$. In contrast to existing results the effects of a heavy charm quark are consistently removed, leaving behind a charmless 3-flavor Lagrangian. This Lagrangian is used to compute the pion and kaon masses to one loop in a regime where the pion mass splitting is large and taken as a leading order effect. In comparison with continuum chiral perturbation theory additional chiral logarithms are present in the results. In particular, chiral logarithms involving the neutral pion mass appear. These predict rather large finite volume corrections in the kaon mass which roughly account for the finite volume effects observed in lattice data.

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I. INTRODUCTION

Lattice simulations with twisted mass (tm) Wilson fermions [1] exhibit various attractive advantages, the most prominent one being automatic $O(a)$ improvement at maximal twist [2]. The European twisted mass collaboration (ETMC) has been performing such simulations for a number of years, both with 2 and 2+1+1 dynamical quark flavors.¹ A major disadvantage of twisted mass terms is the explicit breaking of the flavor and parity symmetries, which results in a mass splitting between the charged and neutral pion masses.

This splitting is a lattice artifact, hence it vanishes in the continuum limit and it is not a fundamental concern. However, the splitting is rather large in practice at the lattice spacings simulated. In particular the $N_f = 2 + 1 + 1$ simulations show a large pion mass splitting. Table 1 of Ref. [4] displays the neutral and charged pion masses for seventeen ensembles generated by the ETMC. In seven ensembles the neutral pion mass is less or about equal to 60% of the charged pion mass, and in four ensembles only the splitting is less than 15%. This is a sizable effect, and it is expected to result in a non-negligible systematic uncertainty.

The impact of the pion mass splitting can be assessed using the appropriate chiral effective theory, so-called tm Wilson ChPT [5–8]. In the ensembles mentioned before the pion mass splitting is a leading order (LO) effect. The consequences of this power counting have been worked out in Ref. [9] for the pion masses and the pion decay constant to one-loop order. The main difference to the familiar continuum ChPT results is the presence of chiral logarithms involving both the charged and the neutral pion mass. If the mass splitting is large the chiral extrapolation is influenced in a nontrivial (but calculable) way.

A related source of systematic uncertainties are the finite volume (FV) effects in the simulations. As already pointed out in Ref. [10] the FV effects are substantially larger if the neutral pion mass is smaller than the charged one. A widely used rule of thumb states that FV effects may be ignored if $M_\pi L$ is equal or greater than 4. Even if this rule is satisfied by the charged pion mass it may be violated significantly by the neutral pion mass. Referring again to table 1 of Ref. [4] we find that 14 out of 17 ensembles satisfy $M_{\pi^\pm} L \geq 3.8$, while at the same time only 6 satisfy $M_{\pi^0} L \geq 3.8$. Three ensembles even have $M_{\pi^0} L \leq 2$. Since the FV effects are dominated by the smallest particle mass one expects large FV effects, much larger than the estimates based on the charged pion mass.

With these cautious remarks in mind it is natural to ask how other observables are affected by a large pion mass splitting. In this paper we give the answer for the simplest observable involving a strange quark, the kaon mass.

Naively one may expect the calculation to be a straightforward extension of the one for the pions in Ref. [9]. This, however, is not the case, for the following reason.

Twisted mass fermions always come in pairs. The $N_f = 2 + 1 + 1$ simulations by ETMC involve dynamical strange and charm quarks, in addition to the light up and down type quarks. The construction of tmWChPT is straightforward only if both fermions of a pair are either light or heavy. In the first case both fermion flavors give rise to pseudo Goldstone bosons in the chiral effective theory, in the latter they only contribute to the low-energy

¹ For a review of these simulations and the obtained results the reader is referred to Ref. [3]

couplings. For the $N_f = 2 + 1 + 1$ case this means that the standard procedure to construct tmWChPT treats the D and D_s mesons as pseudo Goldstone bosons just as the pions and kaons. The construction of this 4-flavor WChPT has been done some time ago [11]. The case of degenerate kaon and D -meson masses has been studied even earlier [12]. However, the results of these papers are valid only for unphysically light charm quarks. They are not applicable to the phenomenologically interesting case with a physical charm quark mass.

The question is how to construct tmWChPT without treating the D mesons as pseudo Goldstone bosons (“charmless ChPT”, for short). The way we proceed here can be summarized as follows. We start with the Lagrangian of 4-flavor ChPT as given in [11]. The expansion in the charm quark mass is subsequently undone by (i) dropping the physical D and D_s meson fields and (ii) absorbing all remaining charm quark dependence in the LECs of the theory. The remaining theory retains only the light degrees of freedom, the pions, kaons and the eta. At the same time the Lagrangian captures correctly all terms in the effective Lagrangian, since the 4-flavor theory we started with contained all terms compatible with the symmetries of $N_f = 2 + 1 + 1$ tm lattice QCD.

This paper is organized as follows. In order not to obscure the essential aspects of the charm removal with technical details we first demonstrate our strategy in continuum ChPT and standard WChPT, where the elimination of the charm quark degrees of freedom is much more transparent. In section III we then apply this procedure to the case with twisted masses and compare our results with the ones obtained in the 4-flavor theory. In section IV we compute the pseudo scalar masses to one-loop order taking the $O(a^2)$ terms in the Lagrangian at LO. As anticipated we find additional chiral logarithms involving the neutral pion. As a first test we compare the predicted FV corrections for the kaon with numerical data generated by ETMC. Section V contains our conclusions. A short account of the results in this paper was already presented in [13].

II. CHPT WITHOUT HEAVY FLAVORS

A. Fixing the notation

The LO chiral Lagrangian (in Euclidean space time) reads

$$\mathcal{L}_2 = \frac{f^2}{4} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle - \frac{f^2}{4} \langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \rangle, \quad (1)$$

where $\langle \dots \rangle$ stands for the trace over flavor indices and the low-energy coefficient (LEC) f is the pseudo scalar decay constant in the chiral limit.² The field $\Sigma = \Sigma(x)$ is an element of

² Our convention is such that $f_\pi = 92.21$ MeV.

$SU(N_f)$ containing the pseudo scalar fields in the usual way,

$$\Sigma(x) = \Sigma_V^{1/2} \Sigma_p(x) \Sigma_V^{1/2}, \quad (2)$$

$$\Sigma_p(x) = \exp \left(\frac{2i}{f} \sum_{a=1}^{N_f^2-1} \pi^a(x) T^a \right). \quad (3)$$

Σ_V denotes the ground state of the theory, defined as the minimum of the potential energy (density). In continuum ChPT it is simply the identity matrix and has no impact. However, for twisted mass terms Σ_V will be non-trivial. The pseudo scalar fields $\pi^a(x)$ are real-valued, and we choose the $SU(N_f)$ group generators to be normalized according to $\text{tr } T^a T^b = \delta^{ab}/2$. The subscript ‘ p ’ in (3) refers to *physical* fields, meaning that the mass terms for the pseudo scalar fields are non-negative and that there are no interaction terms involving less than three pseudo scalars. The parameter χ in the chiral Lagrangian contains the second LO LEC B and the mass matrix M via

$$\chi = 2BM. \quad (4)$$

In the case of two flavors we always take $M = \text{diag}(m, m)$. For the $N_f = 3$ and 4 theories the mass matrix contains m_s and m_c in the obvious way. Note that the mass matrix is usually taken to be diagonal and real. In this case we have $\chi^\dagger = \chi$ and the terms in the chiral Lagrangian simplify slightly. This will no longer be the case for twisted mass terms and we keep the notation general.

The next-to-leading (NLO) Lagrangian is the one given by Gasser and Leutwyler in Ref. [14], although we omit a few terms that are not needed for the calculations in this paper:

$$\begin{aligned} \mathcal{L}_4 = & -L_1 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2 \\ & -L_2 \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \rangle \\ & -L_3 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle^2 \\ & +L_4 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \rangle \\ & +L_5 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger (\chi^\dagger \Sigma + \Sigma^\dagger \chi) \rangle \\ & -L_6 \langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \rangle^2 \\ & -L_7 \langle \chi^\dagger \Sigma - \Sigma^\dagger \chi \rangle^2 \\ & -L_8 \langle \chi^\dagger \Sigma \chi^\dagger \Sigma + \Sigma^\dagger \chi \Sigma^\dagger \chi \rangle. \end{aligned} \quad (5)$$

The coefficients L_i are the well-known Gasser-Leutwyler (GL) coefficients. In $SU(2)$ ChPT some of these terms are redundant and a smaller “operator basis” can be used [15]. However, we prefer to keep this notation because it will make the matching with $SU(3)$ and $SU(4)$ ChPT simpler.

B. Removing charm in ChPT

Before removing charm quark degrees of freedom let us consider a known example, that has already been studied in [14]. Suppose we start off with continuum $SU(3)$ ChPT, but we

are only interested in pionic correlation functions at energies and momenta much below the kaon mass. In this case the kaon and eta meson degrees of freedom "freeze" [14], and we must reproduce the results of SU(2) ChPT.

At the level of the chiral Lagrangian this reduction to SU(2) ChPT is easily derived at tree level. To do so it will be useful to introduce the notation

$$M = \begin{pmatrix} M_2 & \\ & m_s \end{pmatrix}, \quad (6)$$

where M_2 denotes the 2-by-2 mass matrix in the light quark sector. In the field $\Sigma = \Sigma_p$ we ignore the heavy kaon and eta fields by setting them to zero. In that case Σ and its partial derivatives have the form

$$\Sigma = \begin{pmatrix} \Sigma_2 & \\ & 1 \end{pmatrix}, \quad \partial_\mu \Sigma = \begin{pmatrix} \partial_\mu \Sigma_2 & \\ & 0 \end{pmatrix}, \quad (7)$$

where Σ_2 is the field of the SU(2) theory. Using these expressions in \mathcal{L}_2 and \mathcal{L}_4 the kinetic part in the LO Lagrangian and the NLO terms proportional to L_1, L_2 and L_3 reduce to their SU(2) counterparts, while terms without derivatives produce extra terms. For example, the trace part in the mass term reduces to the sum $\langle M^\dagger \Sigma + \Sigma^\dagger M \rangle = \langle \Sigma_2 M_2^\dagger + \Sigma_2^\dagger M_2 \rangle + 2m_s$. Hence, the SU(3) mass term reduces to the SU(2) mass term plus an irrelevant constant that can be dropped.³

Non-trivial extra contributions stem from the NLO terms in the chiral Lagrangian. The L_4 term also separates into a sum of two terms. One is the L_4 term in the SU(2) theory, while the second one reads $4Bm_s L_4 \langle \partial_\mu \Sigma_2 \partial_\mu \Sigma_2^\dagger \rangle$. This has the form of the kinetic term in \mathcal{L}_2 , and combining these two we reproduce the kinetic term in the SU(2) theory provided we identify

$$f_{(2)} = f \left(1 + 8 \frac{Bm_s}{f^2} L_4 \right) \quad (8)$$

with the LO LEC $f_{(2)}$ of SU(2) ChPT. In a similar fashion one can reduce all NLO terms in the chiral Lagrangian. Most of them reduce to the corresponding SU(2) terms plus irrelevant constants. An exception is the contribution proportional to L_6 , which spawns the contribution $-8L_6 Bm_s \langle \chi_2^\dagger \Sigma_2 + \Sigma_2^\dagger \chi_2 \rangle$. This has the form of the mass term in the LO Lagrangian. Combining both and requiring the sum to be equivalent to the SU(2) mass term we can read off the second LO LEC $B_{(2)}$ in the SU(2) theory,

$$B_{(2)} = B \left(1 + 16 \frac{Bm_s}{f^2} (2L_6 - L_4) \right). \quad (9)$$

The results (8) and (9) are not new and can already be found in the paper of Gasser and Leutwyler, cf. eqs. (11.2) and (11.3) of [14]. They display the leading analytic dependence

³ We refer to constants as terms without Σ fields. Thinking of the strange quark mass as an adjustable parameter in lattice QCD simulations these terms are not constant in a strict sense.

of the LECs on the strange quark mass. Recall that SU(3) ChPT is an expansion around $m_u = m_d = m_s = 0$, while SU(2) ChPT expands around $m_u = m_d = 0$ and $m_s \neq 0$. The full relation between the SU(2) and SU(3) LECs involve non-analytic chiral logarithms as well. The main point here is that we can undo the expansion in the strange quark mass and recover the SU(2) theory provided we absorb some remnant strange quark mass dependence in the LECs. Schematically we write this as

$$\mathcal{L}_{\text{chiral}}^{\text{SU}(3)}(f, B) \rightarrow \mathcal{L}_{\text{chiral}}^{\text{SU}(2)}(f_{(2)}, B_{(2)}) + \text{constants}, \quad (10)$$

where the arrow indicates the use of the reduced fields in (7).

The same procedure is easily applied to the reduction of SU(4) ChPT and the removal of the charm quark degrees of freedom. In SU(4) ChPT the field Σ is a 4-by-4 matrix and the index a in (3) runs from 1 to 15. If the charm quark mass were sufficiently small the additional pseudo scalars would be the D mesons, made of a charm and a light quark, the D_s meson, made of a charm and a strange quark, and the η_{15} , an additional neutral flavor non-singlet pseudo scalar. The LO masses of these particles are easily found and read [11]

$$m_D^2 = B(m + m_c), \quad m_{D_s}^2 = B(m_s + m_c). \quad (11)$$

Due to mixing the η_8 the η_{15} are not mass eigenstates, and the diagonalization of a 2-by-2 mass matrix is required to compute the masses [11]. These are not needed in the following.

Similarly to (6) and (7) we introduce

$$M = \begin{pmatrix} M_3 & \\ & m_c \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma_3 & \\ & 1 \end{pmatrix}. \quad (12)$$

M_3 is the mass matrix in the 3-flavor theory, i.e. $M_3 = \text{diag}(m, m, m_s)$. In $\Sigma = \Sigma_p$ we drop the heavy fields associated with the charm quark flavor, i.e. in (3) the sum over a runs from 1 to 8 only. With this notation the matching of the SU(4) theory to the SU(3) one is essentially the same as in the last section, provided we replace m_s by m_c in the formulae. Therefore, the final results for the m_c dependent LO LECs in the 3-flavor theory read

$$f_{(3)} = f \left(1 + 8 \frac{Bm_c}{f^2} L_4 \right), \quad (13)$$

$$B_{(3)} = B \left(1 + 16 \frac{Bm_c}{f^2} (2L_6 - L_4) \right), \quad (14)$$

and the summarizing result (10) translates into

$$\mathcal{L}_{\text{chiral}}^{\text{SU}(4)}(f, B) \rightarrow \mathcal{L}_{\text{chiral}}^{\text{SU}(3)}(f_{(3)}, B_{(3)}) + \text{constants}. \quad (15)$$

There is an important difference to the previously discussed removal of the strange quark. The strange quark mass is sufficiently small such that the expansion in m_s works reasonably well, and the matching formulae (8), (9) between the LECs are valid and useful. In contrast, the physical charm quark mass is much too heavy for an expansion in m_c , and the analogous results (13), (14) are of no interest. Still, the main point here is that the procedure described

above provides the correct right hand side in (15) even if the chiral expansion of the left hand side is poor due to a charm quark that is too heavy. The reason is that chiral symmetry and its particular breaking by a mass term restricts the number and form of the terms in the chiral Lagrangian, irrespectively of how heavy the mass is. The size of the mass just determines how well the expansion in powers of this mass works.

Obviously there is no need to construct SU(3) ChPT the way we have done it here. We can directly formulate the chiral effective theory that contains only the degrees of freedom that are sufficiently light. However, for twisted mass lattice QCD the construction described here is a viable procedure to derive the 3-flavor chiral Lagrangian, in particular since the chiral Lagrangian including charm is known.

C. Removing charm in Wilson ChPT

Wilson ChPT (WChPT) [5] is an extension of continuum ChPT.⁴ In addition to expanding in small momenta and pseudo scalar masses one also expands in small lattice spacings a around the continuum limit $a = 0$. The Lagrangian of WChPT has been constructed through $O(a^2)$ and is well known [18, 19]. In the following we want to remove charm from 4-flavor WChPT and check whether we obtain the expected 3-flavor theory. As we will see this is not quite the case. The heavy charm quark leaves behind a trace in the 3-flavor theory, but this remnant is expected.

We first summarize the terms of $O(a)$ and $O(a^2)$ in the chiral Lagrangian. At LO in the lattice spacing there is only one term [18],

$$\mathcal{L}_a = -\frac{f^2}{4}\rho\langle\Sigma + \Sigma^\dagger\rangle. \quad (16)$$

It has the form of a mass term with χ replaced by

$$\rho = 2W_0a. \quad (17)$$

W_0 is a LEC of mass dimension 3, such that ρ has mass dimension 2, just as χ . However, ρ is flavor diagonal and real, hence it can be taken out of the trace in flavor space.

Since the term (16) is essentially a mass term it is convenient to absorb it in a redefinition of the quark mass matrix. Explicitly, we define the so-called shifted mass matrix M' by [5]

$$\chi' = \chi + \rho \quad \Leftrightarrow \quad M' = M + \frac{W_0}{B}a. \quad (18)$$

With this definition the mass term and the $O(a)$ term combine to a mass term with the shifted mass parameter χ' . This parameter, as a spurion field, has the same transformation properties as the original χ . For the construction of higher order terms in the chiral Lagrangian one can use either (χ, ρ) or (χ', ρ) . In the following we always assume the latter set of parameters, and from now on we drop the prime on the shifted mass, since we exclusively deal with it in the following.

⁴ For an introduction to Wilson ChPT see [16, 17].

At higher order there are terms of $O(ap^2, aM, a^2)$ [18, 19],

$$\begin{aligned}
\mathcal{L}_{ap^2} &= W_4 \rho \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \langle \Sigma + \Sigma^\dagger \rangle \\
&\quad + W_5 \rho \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger (\Sigma + \Sigma^\dagger) \rangle, \\
\mathcal{L}_{aM} &= -W_6 \rho \langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \rangle \langle \Sigma + \Sigma^\dagger \rangle \\
&\quad - W_7 \rho \langle \chi^\dagger \Sigma - \Sigma^\dagger \chi \rangle \langle \Sigma - \Sigma^\dagger \rangle \\
&\quad - W_8 \rho \langle \chi^\dagger \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \chi \rangle, \\
\mathcal{L}_{a^2} &= -W'_6 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \\
&\quad - W'_7 \rho^2 \langle \Sigma - \Sigma^\dagger \rangle^2 \\
&\quad - W'_8 \rho^2 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle.
\end{aligned} \tag{19}$$

The coefficients W_i, W'_i are dimensionless LECs, just as the Gasser-Leutwyler coefficients.

It is straightforward to perform the removal of charm as described in the previous section. The goal is to identify those terms that need to be absorbed in the LECs. These are the $O(m_c, m_c^2, am_c)$ terms. Terms of $O(a, a^2)$ should be left explicit, even though they can be absorbed. In order to give an example consider the W_4 term in (19). Using $\langle \Sigma + \Sigma^\dagger \rangle = \langle \Sigma_3 + \Sigma_3^\dagger \rangle + 2$ the W_4 term splits into the sum $W_4 \rho \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle \langle \Sigma_3 + \Sigma_3^\dagger \rangle + 2W_4 \rho \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle$. The first part is just the W_4 term in the 3-flavor theory. The second one has the form of the kinetic term. In principle we could absorb this contribution in the definition of $f_{(3)}$ in the 3-flavor theory, similarly to what we have done before with the $O(m_c)$ effects. However, we do not want to do this. After all, the goal of WChPT is to expand around $a = 0$ with explicit dependence on the lattice spacing, so all $O(a)$ terms should remain explicit.

Performing the substitution (12) in (19) we obtain the following list of terms (up to irrelevant constants that we have dropped):

$$\begin{aligned}
\mathcal{L}_{ap^2} &= +W_4 \rho \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle \langle \Sigma_3 + \Sigma_3^\dagger \rangle \\
&\quad + W_5 \rho \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger (\Sigma_3 + \Sigma_3^\dagger) \rangle \\
&\quad + 2W_4 \rho \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle, \\
\mathcal{L}_{aM} &= -W_6 \rho \langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \rangle \langle \Sigma_3 + \Sigma_3^\dagger \rangle \\
&\quad - W_7 \rho \langle \chi_3^\dagger \Sigma_3 - \Sigma_3^\dagger \chi_3 \rangle \langle \Sigma_3 - \Sigma_3^\dagger \rangle \\
&\quad - W_8 \rho \langle \chi_3^\dagger \Sigma_3 \Sigma_3 + \Sigma_3^\dagger \Sigma_3^\dagger \chi_3 \rangle \\
&\quad - 2W_6 \rho \langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \rangle - 4W_6 B m_c \rho \langle \Sigma_3 + \Sigma_3^\dagger \rangle, \\
\mathcal{L}_{a^2} &= -W'_6 \rho^2 \langle \Sigma_3 + \Sigma_3^\dagger \rangle^2 \\
&\quad - W'_7 \rho^2 \langle \Sigma_3 - \Sigma_3^\dagger \rangle^2 \\
&\quad - W'_8 \rho^2 \langle \Sigma_3 \Sigma_3 + \Sigma_3^\dagger \Sigma_3^\dagger \rangle \\
&\quad - 4W'_6 \rho^2 \langle \Sigma_3 + \Sigma_3^\dagger \rangle.
\end{aligned} \tag{20}$$

The W_6 and W'_6 terms have spawned additional mass terms proportional to $\langle \Sigma_3 + \Sigma_3^\dagger \rangle$ that

can again be absorbed in a shifted mass. Explicitly we define

$$\chi_3'' = \chi_3 + \frac{16Bm_c}{f^2}W_6\rho + \frac{16}{f^2}W_6'\rho^2. \quad (21)$$

The term proportional to the charm quark mass is in the end a redefinition of the LEC W_0 . Recall that χ_3 already includes the leading shift proportional to ρ , cf. (18). In terms of the original mass M we can write the combined shifted mass as

$$M_3'' = M_3 + \frac{W_{0,(3)}}{B}a + \frac{16W_0W_6'\rho}{Bf^2}a, \quad (22)$$

where we introduced

$$W_{0,(3)} = W_0 \left(1 + 16\frac{Bm_c}{f^2}W_6 \right). \quad (23)$$

As before the heavy charm quark effects are included in the LECs. Finally, in order to express everything in terms of this modified $W_{0,(3)}$ it should be used in the definition of ρ which amounts in a redefinition of the other NLO LECs. For example, the requirement $W_0^2\tilde{W}_6' = W_{0,(3)}^2\tilde{W}_6'$ defines the LEC \tilde{W}_6' . In the end the relevant terms in the chiral Lagrangian are

$$\begin{aligned} \mathcal{L}_{ap^2} &= +W_4\rho\langle\partial_\mu\Sigma_3\partial_\mu\Sigma_3^\dagger\rangle\langle\Sigma_3+\Sigma_3^\dagger\rangle \\ &\quad +W_5\rho\langle\partial_\mu\Sigma_3\partial_\mu\Sigma_3^\dagger(\Sigma_3+\Sigma_3^\dagger)\rangle \\ &\quad +2W_4\rho\langle\partial_\mu\Sigma_3\partial_\mu\Sigma_3^\dagger\rangle, \\ \mathcal{L}_{aM} &= -W_6\rho\langle\chi_3^\dagger\Sigma_3+\Sigma_3^\dagger\chi_3\rangle\langle\Sigma_3+\Sigma_3^\dagger\rangle \\ &\quad -W_7\rho\langle\chi_3^\dagger\Sigma_3-\Sigma_3^\dagger\chi_3\rangle\langle\Sigma_3-\Sigma_3^\dagger\rangle \\ &\quad -W_8\rho\langle\chi_3^\dagger\Sigma_3\Sigma_3+\Sigma_3^\dagger\Sigma_3^\dagger\chi_3\rangle \\ &\quad -2W_6\rho\langle\chi_3^\dagger\Sigma_3+\Sigma_3^\dagger\chi_3\rangle, \\ \mathcal{L}_{a^2} &= -W_6'\rho^2\langle\Sigma_3+\Sigma_3^\dagger\rangle^2 \\ &\quad -W_7'\rho^2\langle\Sigma_3-\Sigma_3^\dagger\rangle^2 \\ &\quad -W_8'\rho^2\langle\Sigma_3\Sigma_3+\Sigma_3^\dagger\Sigma_3^\dagger\rangle, \end{aligned} \quad (24)$$

where we reverted to the old notation for the LECs without a tilde. Except for two terms proportional to W_4 and W_6 these are just the terms in the 3-flavor chiral Lagrangian. In analogy to (15) we can summarize our results by

$$\begin{aligned} \mathcal{L}_{\text{Wilson}}^{\text{SU}(4)}(f, B, W_0) &\rightarrow \mathcal{L}_{\text{Wilson}}^{\text{SU}(3)}(f_{(3)}, B_{(3)}, W_{0,(3)}) + 2W_4\rho\langle\partial_\mu\Sigma_3\partial_\mu\Sigma_3^\dagger\rangle \\ &\quad -2W_6\rho\langle\chi_3^\dagger\Sigma_3+\Sigma_3^\dagger\chi_3\rangle + \text{constants}. \end{aligned} \quad (25)$$

In contrast to the continuum ChPT result we find here two additional contributions in the effective 3-flavor theory. A heavy charm quark leaves behind a remnant no matter how heavy it is. This perhaps counter intuitive result can be understood better by going back to

the Symanzik effective theory that underlies WChPT [20]. The $O(a)$ effects stem entirely from the Pauli term in the Symanzik effective action

$$S_{\text{Pauli}} = a \int d^4x \sum_{f=u,d,\dots} \bar{\psi}_f \sigma_{\mu\nu} F^{\mu\nu} \psi_f. \quad (26)$$

Here the gluon field strength tensor acts in color space, while $\sigma_{\mu\nu}$ acts in Dirac space. In flavor space the Pauli term is diagonal, hence it is a sum over the individual flavor contributions. Note that this term is independent of the quark masses, so a charm quark contributes lattice artifacts irrespectively of how heavy it is. These artifacts contribute to $O(a)$ effects in WChPT that stem from the charm quark but come without the dependence on the charm quark mass.

For later reference we mention that the results of this section are essentially unaltered if we remove both charm and strange from the 4-flavor theory. In that case (25) changes slightly to

$$\begin{aligned} \mathcal{L}_{\text{WChPT}}^{\text{SU}(4)}(f, B, W_0) &\rightarrow \mathcal{L}_{\text{WChPT}}^{\text{SU}(2)}(f_{(2)}, B_{(2)}, W_{0,(2)}) + 4W_4\rho\langle\partial_\mu\Sigma_2\partial_\mu\Sigma_2^\dagger\rangle \\ &\quad - 4W_6\rho\langle\chi_2^\dagger\Sigma_2 + \Sigma_2^\dagger\chi_2\rangle + \text{constants}. \end{aligned} \quad (27)$$

Removing the strange quark leaves the same remnant behind as charm, so the two additional terms are twice as big.

III. CHARMLESS TWISTED MASS WILSON CHPT

A. Ground state and physical fields in 4-flavor tmWChPT

In the following we are going to follow the steps of the last section for the removal of charm, this time for the 4-flavor theory with twisted mass terms. There is one additional complication, namely the identification of the physical degrees freedom we want to remove. In tmWChPT this implies finding the non-trivial ground (or vacuum) state Σ_V of the theory, defined as the minimum of the potential energy (density).

In the following we always assume the twisted mass term in the 4-flavor theory to be of the form

$$M = \begin{pmatrix} M_l & 0 \\ 0 & M_h \end{pmatrix}, \quad (28)$$

where both submatrices M_l, M_h are 2-by-2 matrices and explicitly given by [21, 22]

$$M_l = m + i\sigma^3\mu_l, \quad (29)$$

$$M_h = m + i\sigma^1\mu_h + \delta\sigma^3. \quad (30)$$

The σ^a denote the usual Pauli matrices. This particular mass term corresponds to the so-called perpendicular choice according to Ref. [23], and it is usually employed by the ETMC in their numerical simulations [24]. It leads to a real fermion determinant [22] and has a symmetry that guarantees degenerate masses for all kaons [25].

The chiral Lagrangian of 4-flavor tmWChPT is easily constructed and can be found in Ref. [11]. The only difference to the formulae in the last section is the twisted mass term (28) entering the definition of χ and χ' in eqs. (4) and (18), respectively. The number and form of the terms in $\mathcal{L}_2, \mathcal{L}_4$ and \mathcal{L}_{aM} remain unchanged [11].

Before looking for the ground state we need to specify a power counting scheme. To most of the generated lattice data the so-called *generically small quark mass* (GSM) regime [8] applies, where the terms associated with the nonzero lattice spacing contribute at NLO in the chiral expansion. The LO Lagrangian consists of the continuum parts only, $\mathcal{L}_{\text{LO}} = \mathcal{L}_2$. This implies, that the LO potential energy stems from the mass term only and reads

$$V_{\text{LO}} = \frac{f^2 B}{2} \langle M^\dagger \Sigma + \Sigma^\dagger M \rangle. \quad (31)$$

The mass matrix (28) is block diagonal. This implies that the vacuum state will be block diagonal as well. Making the ansatz

$$\Sigma_V = \begin{pmatrix} \Sigma_l & 0 \\ 0 & \Sigma_h \end{pmatrix} \quad (32)$$

with the two-dimensional submatrices Σ_l and Σ_h , the potential energy separates into a sum of two contributions, $V_{\text{LO}} = V_l + V_h$. Each of them is the known potential of 2-flavor tmWChPT. This potential has been discussed at length in the literature [7, 26, 27] and we can carry over the results. The ground states in the light and heavy sector point into the direction of the corresponding twisted masses,

$$\Sigma_l = e^{i\omega_l \sigma^3}, \quad \Sigma_h = e^{i\omega_h \sigma^1}. \quad (33)$$

The angles ω_l and ω_h are the light and heavy vacuum angle, respectively, and to LO the potential is minimized for

$$\cot \omega_l = \frac{m}{\mu_l}, \quad \cot \omega_h = \frac{m}{\mu_h}. \quad (34)$$

Maximal twist $\omega_{l,h} = \pi/2$ is achieved by setting the shifted mass m to zero.

The main observation here is that the ground state Σ_V is in general non-trivial and needs to be taken into account in the definition of Σ in (2). However, in many terms of the chiral Lagrangian it does not contribute. For instance, in the kinetic term the ground state drops out exactly, $\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle = \langle \partial_\mu \Sigma_p \partial_\mu \Sigma_p^\dagger \rangle$. Similarly, the ground state does not contribute to the NLO terms proportional to L_1, L_2, L_3 . The cancellation of Σ_V does not work in the traces involving the mass M , since M does not commute with Σ_V . To see this consider $\langle M \Sigma^\dagger \rangle$, one part of the mass term in the chiral Lagrangian. Here the ground state is absorbed in the definition of the physical mass, i.e.

$$\langle M \Sigma^\dagger \rangle = \langle M_p \Sigma_p^\dagger \rangle, \quad M_p = (\Sigma_V^\dagger)^{1/2} M (\Sigma_V^\dagger)^{1/2}. \quad (35)$$

The physical mass matrix M_p is block diagonal as M , so the light and heavy sectors can be studied separately. For the light sector we again find the result known from 2-flavor WChPT,

$$M_{l,p} = m'_l, \quad m'_l = \sqrt{m^2 + \mu_l^2}. \quad (36)$$

The light physical mass matrix is flavor diagonal and m'_l denotes the usual (light) ‘radial mass’. The interpretation of this result is that the twisted mass term in the light sector is equivalent to a standard degenerate mass term, and we can conclude that the degenerate physical up and down type quark mass is equal to the light radial mass.⁵

For the heavy sector we find

$$M_{h,p} = m'_h + \delta\sigma^3, \quad m'_h = \sqrt{m^2 + \mu_h^2}. \quad (37)$$

Here too the twisted mass term is equivalent to a standard mass term but the physical quark masses are not degenerate. Instead, we find the correspondence⁶

$$m_s = m'_h + \delta, \quad m_c = m'_h - \delta. \quad (38)$$

We are interested in the regime with a large charm quark mass keeping the strange quark mass small. Eq. (38) tells us that this is obtained for m'_h and $-\delta$ being large while the difference of these parameters needs to be kept small. Recall that $m'_h = \mu_h$ at maximal twist, so the heavy twisted mass is large for heavy charm quarks. Note that this constraint simplifies the tuning to maximal twist in the heavy sector, since tuning to $\omega_h \approx \pi/2$ is easier the larger the denominator is in (34).

Working to NLO the LO ground state is sufficient for the expansion of the NLO Lagrangian in terms of physical fields. The NLO ground state is needed only in the LO mass term where it spawns an additional interaction term at NLO. Even though this term is not needed for the calculations in this paper let us discuss it briefly for completeness.

The potential at NLO contains, in addition to V_{LO} , higher order terms from the NLO Lagrangian. These result in a small shift of the vacuum angles [8, 11],

$$\omega_l^{\text{NLO}} = \omega_l + \epsilon_l, \quad \omega_h^{\text{NLO}} = \omega_h + \epsilon_h, \quad (39)$$

with ω_l, ω_h being the LO angles. Using the NLO angles in (33) and the NLO ground state in the mass term in \mathcal{L}_2 we find, to linear order in the small corrections ϵ_l, ϵ_h , the contribution

$$\mathcal{L}_{2,\epsilon} = -\frac{f^2 B}{4} \langle \{\hat{\epsilon}, M_p\} i(\Sigma_p - \Sigma_p^\dagger) \rangle, \quad \hat{\epsilon} = \begin{pmatrix} \epsilon_l \sigma_3 & 0 \\ 0 & \epsilon_h \sigma_1 \end{pmatrix}. \quad (40)$$

Here $\{\hat{\epsilon}, M_p\}$ denotes the anti-commutator of the matrix $\hat{\epsilon}$ and the physical (hence Hermitian) quark mass matrix. Expanding in pseudo scalar fields this contribution results in interaction terms with an odd number of pseudo scalar fields. The terms linear in the pseudo scalar fields are eventually cancelled by corresponding terms of the NLO Lagrangian, a simple consequence of the fact that we expand around the minimum of the action. The actual

⁵ The pion mass splitting between the charged and neutral pions is an $\mathcal{O}(a^2)$ effect caused by \mathcal{L}_{a^2} , a term at NLO in the GSM regime and so far not being taken into account.

⁶ In order to get the correct relative size of these two masses the parameter δ needs to be negative. Our sign convention for δ agrees with the one used by the ETMC.

values for ϵ_l, ϵ_h have already been calculated in Ref. [11] and read⁷

$$\epsilon_l = -\frac{8}{f^2} \frac{\rho \sin \omega_l}{2Bm'_l} [2Bm'_l W_{68} + 2Bm'_h 2W_6 + \rho \cos \omega_l 2W'_{68} + \rho \cos \omega_h 4W'_6], \quad (41)$$

$$\epsilon_h = -\frac{8}{f^2} \frac{\rho \sin \omega_h}{2Bm'_h} [2Bm'_h W_{68} + 2Bm'_l 2W_6 + \rho \cos \omega_h 2W'_{68} + \rho \cos \omega_l 4W'_6]. \quad (42)$$

Here we introduced the short hand notation $W_{68} = 2W_6 + W_8$ and $W'_{68} = 2W'_6 + W'_8$.

B. The charmless 3-flavor theory

It is now straightforward to follow section II and remove the charm quark degrees of freedom from the theory. To quote our results we begin with the continuum part $\mathcal{L}_{\text{cont}} = \mathcal{L}_2 + \mathcal{L}_4$. As we have seen in the previous subsection, the entire effect of the ground state is to bring the twisted quark mass into its physical (i.e. diagonal) form. Once this is achieved the reduction of fields on the right hand side works as before, and the result can be summarized by

$$\mathcal{L}_{\text{cont}}^{\text{SU}(4)}(f, B, M, \Sigma) = \mathcal{L}_{\text{cont}}^{\text{SU}(4)}(f, B, M_p, \Sigma_p) \rightarrow \mathcal{L}_{\text{cont}}^{\text{SU}(3)}(f_{(3)}, B_{(3)}, M_p, \Sigma_p) + \text{constants}. \quad (43)$$

The nontrivial part to write down are the terms of $O(a)$ and $O(a^2)$ given in (19). The reason is that a remnant of the ground state remains in the terms without the mass matrix. It is useful to introduce

$$\tilde{\Sigma}_l = \begin{pmatrix} \Sigma_l & 0 \\ 0 & \cos \omega_h \end{pmatrix}, \quad (44)$$

which is the upper-left 3-by-3 matrix of the ground state in (32). This is effectively the ground state of the 3-flavor theory once the charm degrees of freedom are removed. In terms of this ground state the 3-flavor chiral Lagrangians read (dropping irrelevant constants)

$$\begin{aligned} \mathcal{L}_{ap^2} &= +W_4 \rho \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle \langle \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle \\ &\quad + W_5 \rho \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger (\Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger) \rangle \\ &\quad + 2W_4 \rho \cos \omega_h \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle, \\ \mathcal{L}_{aM} &= -W_6 \rho \langle \chi_3 (\Sigma_3 + \Sigma_3^\dagger) \rangle \langle \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle \\ &\quad - W_7 \rho \langle \chi_3 (\Sigma_3 - \Sigma_3^\dagger) \rangle \langle \Sigma_3 \tilde{\Sigma}_l - \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle \\ &\quad - W_8 \rho \langle \chi_3 (\Sigma_3 \tilde{\Sigma}_l \Sigma_3 + \Sigma_3^\dagger \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger) \rangle \\ &\quad - 2W_6 \rho \cos \omega_h \langle \chi_3 (\Sigma_3 + \Sigma_3^\dagger) \rangle, \end{aligned}$$

⁷ Note that our notation for the LECs differs from the one used in Ref. [11], which makes a comparison of our results with eqs. (4.2) and (4.3) of [11] a nuisance.

$$\begin{aligned}
\mathcal{L}_{a^2} = & -W'_6\rho^2 \langle \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle^2 \\
& -W'_7\rho^2 \langle \Sigma_3 \tilde{\Sigma}_l - \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle^2 \\
& -W'_8\rho^2 \langle (\Sigma_3 \tilde{\Sigma}_l)^2 + (\tilde{\Sigma}_l^\dagger \Sigma_3^\dagger)^2 \rangle \\
& -4W'_6\rho^2 \cos \omega_h \langle \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle \\
& +2W'_8\rho^2 \sin^2 \omega_h \langle P_s (\Sigma_3 + \Sigma_3^\dagger) \rangle.
\end{aligned} \tag{45}$$

In the last line we introduced the matrix $P_s = \text{diag}(0, 0, 1)$, which can be interpreted as the projector onto the strange quark sector.

The results (45) are the twisted mass analogues of the results (24) for untwisted Wilson fermions. In fact, we need to reproduce these results exactly if we set the twisted quark masses μ_l, μ_h to zero. Since in that case $\omega_l = \omega_h = 0$ and $\tilde{\Sigma}_l = 1$ this is indeed the case.⁸ However, note that the last term in (45) has no analogue in (24) since it vanishes for $\omega_h = 0$.

Let us also consider the case where we remove the strange quark too. This can be done in two different ways. We either start from the 4-flavor theory and restrict the physical fields to the pions. Alternatively, we can restrict Σ_3 in (45) to the pions. Both ways lead to the same result, which can be written as

$$\begin{aligned}
\mathcal{L}_{\text{tmWChPT}}^{\text{SU}(4)}(f, B, W_0) \rightarrow & \mathcal{L}_{\text{tmWChPT}}^{\text{SU}(2)}(f_{(2)}, B_{(2)}, W_{0,(2)}) + 4W_4\rho \cos \omega_h \langle \partial_\mu \Sigma_2 \partial_\mu \Sigma_2^\dagger \rangle \\
& -4W_6\rho \cos \omega_h \langle \chi_2^\dagger \Sigma_2 + \Sigma_2^\dagger \chi_2 \rangle + \text{constants}.
\end{aligned} \tag{46}$$

This is the same result as for untwisted WChPT, cf. (27), except for the simple replacement $\rho \rightarrow \rho \cos \omega_h$.

This result has an important implication. Once we tune to maximal twist in the heavy sector the two extra terms proportional to W_4 and W_6 vanish. Only the familiar chiral Lagrangian for SU(2) tmWChPT remains. This chiral Lagrangian is therefore appropriate to describe pion physics even for $N_f = 2 + 1 + 1$ lattice data. This fact has been implicitly assumed in Ref. [9], where results for the pion masses and the pion decay constant, obtained in 2-flavor tmWChPT, were used in analyzing $N_f = 2 + 1 + 1$ flavor lattice data.

C. Light vacuum angle and tree level masses in the charmless 3-flavor theory

As further checks for our main result (45) we compute, in the GSM regime, the light vacuum angle ω_l and the tree level pseudo scalar masses and compare the results with the ones obtained in the 4-flavor theory. This comparison is illuminating in so far as it explicitly demonstrates the essence of our charmless 3-flavor theory: The effects of the heavy charm quark only are removed, while the corrections due to the light pseudo scalars are correctly reproduced.

In the GSM regime the LO Lagrangian contains just the continuum part \mathcal{L}_2 . This is the case in the 4-flavor theory and it is not changed when we remove charm. This implies that

⁸ The extra term $-4W'_6\rho^2 \langle \Sigma_3 + \Sigma_3^\dagger \rangle$ in (45) that is missing in (24) corresponds to the last term in (20) that we absorbed in the shifted mass.

the LO results (33), (34) for Σ_l also hold in the 3-flavor theory. Deviations show up at NLO in the correction ϵ_l . Computing this correction based on the potential energy stemming from (45) we obtain

$$\epsilon_l = -\frac{8}{f^2} \frac{\rho \sin \omega_l}{2Bm'_l} [2Bm'_l W_{68} + 2Bm_s W_6 + \rho \cos \omega_l 2W'_{68} + \rho \cos \omega_h 4W'_6], \quad (47)$$

This agrees with the result of the 4-flavor theory in (41) except for the replacement $m'_h \rightarrow m_s/2$. This is exactly what we expect. According to (38) we can write $m'_h = (m_c + m_s)/2$. The charm quark mass contribution is absorbed in the LECs of the 3-flavor theory. This leaves behind the part proportional to $m_s/2$ as in (47). However, note that all the other terms in ϵ_l are correctly reproduced in the 3-flavor theory. Also note that the 4-flavor result (41) is valid only for sufficiently small charm quark masses such that ϵ_l is a small correction to the LO vacuum angle. Such a restriction on the charm mass is not necessary for (47).

To NLO in the GSM regime the pseudo scalar masses are of the form

$$M_{\text{GB,NLO}}^2 = M_{\text{GB,NLO,cont}}^2 + \Delta M_{\text{GB},a}^2. \quad (48)$$

The first part refers to the familiar NLO result of continuum ChPT [14]. The second part contains all the corrections associated with the nonzero lattice spacing, originating in (45). Expanding to quadratic order in the pion fields it is straightforward to obtain the correction to the charged pion mass,

$$\begin{aligned} \Delta M_{\pi^\pm,a}^2 = & \frac{8}{f^2} \left(\rho m_\pi^2 \cos \omega_l [2W_{68} - W_{45}] \right. \\ & + \rho(2m_K^2 - m_\pi^2) \cos \omega_l W_6 \\ & + \rho m_\pi^2 \cos \omega_h [2W_6 - 2W_4] \\ & + \rho^2 \cos^2 \omega_l [4W'_6 + 2W'_8] \\ & \left. + \rho^2 \cos \omega_l \cos \omega_h 4W'_6 \right). \end{aligned} \quad (49)$$

Here we introduced the abbreviation $W_{ij} = 2W_i + W_j$, and the mass dependence is parametrized in terms of the LO masses, $m_\pi^2 = 2Bm'_l$, $m_K^2 = B(m_s + m'_l)$. The analogous result for the kaon mass correction reads

$$\begin{aligned} \Delta M_{K,a}^2 = & \frac{4}{f^2} \left(\rho m_K^2 (\cos \omega_l + \cos \omega_h) [8W_6 + 2W_8 - 4W_4 - W_5] \right. \\ & - \rho(2m_K^2 - m_\pi^2) (\cos \omega_l + \cos \omega_h) W_6 \\ & + \rho^2 (\cos \omega_l + \cos \omega_h)^2 [4W'_6 + W'_8] \\ & \left. - \rho^2 (\sin^2 \omega_l + \sin^2 \omega_h) W'_8 \right). \end{aligned} \quad (50)$$

By construction, both results do not depend explicitly on the charm quark mass. Comparing to the corresponding results in the 4-flavor theory we find again a simple (and expected) substitution rule to obtain our 3-flavor results. Replacing the tree level masses in [11] according to

$$\left. \begin{aligned} m_{D_s}^2 &= B(m_s + m_c) \\ -(m_D^2 - m_K^2) &= B(m_s - m_c) \end{aligned} \right\} \rightarrow Bm_s = (2m_K^2 - m_\pi^2)/2. \quad (51)$$

we recover our results (49) and (50). This demonstrates once more that the charmless 3-flavor theory removes the charm quark dependence completely, while the effects due to the light degrees of freedom are kept and unchanged.

IV. PSEUDO SCALAR MASSES IN THE LCE REGIME

A. Preliminaries

Besides the GSM regime a second power counting scheme is frequently discussed in the literature, the so-called Aoki or *large cut-off effects* (LCE) regime [8, 28, 29]. This regime assumes that the $O(a^2)$ cut-off effects in the chiral expansion are of the same order as the effects due to the quark masses. More precisely, it assumes that \mathcal{L}_{a^2} contributes to LO in the effective Lagrangian,

$$\mathcal{L}_{\text{LO}} = \mathcal{L}_2 + \mathcal{L}_{a^2}. \quad (52)$$

The $O(a^2)$ term leads to the mass splitting between the charged and the neutral pion [30]. This splitting is a LO effect in the LCE regime counting, which is the appropriate one if the size of the splitting is observed to be of the same order as the charged pion mass. As discussed in the introduction this is indeed the case for a substantial part of the ETMC data.

Taking \mathcal{L}_{a^2} at LO results in interaction vertices of $O(a^2)$. These contribute to the pseudo scalar masses at one loop, as we show in this section. The calculation follows the one in Ref. [9], where the pion masses are computed in the 2-flavor theory. The reader is referred to this reference for aspects of the calculation that are independent of the number of flavors. In particular, we work at maximal twist only. This simplifies the calculation significantly and it is the relevant case for practical applications.

In the following we exclusively work with the charmless 3-flavor Lagrangian. To simplify the notation we drop the subscripts $_{(3)}$ in the LO LECs of the 3-flavor theory and simply use f and B from now on.

B. Tree level masses and vertices

Our LO Lagrangian is as in (52) with \mathcal{L}_{a^2} given in (45). We assume maximal twist in both the heavy and the light sector, i.e. $\omega_l = \omega_h = \pi/2$. This is achieved by setting the untwisted shifted mass m to zero, see eq. (34). This implies that the radial masses in both the heavy and the light sector are determined by the respective twisted masses, i.e. $m'_{l,h} = \mu_{l,h}$.

At maximal twist the ground state reduces to $\tilde{\Sigma}_l = \text{diag}(i\sigma^3, 0)$ and the tree level pseudo scalar masses are easily computed. The pion masses reproduce the familiar 2-flavor results

[7, 8, 30],

$$m_{\pi^\pm}^2 = 2B\mu_l \quad (53)$$

$$m_{\pi^0}^2 = m_{\pi^\pm}^2 + \Delta m_\pi^2,$$

$$\Delta m_\pi^2 = -\frac{16\rho^2}{f^2}W'_{68}. \quad (54)$$

The $N_f = 2$ literature very often uses a different convention for the LECs appearing in the mass splitting. Introducing $c_2 = -64W'_{68}W_0^2/f^2$ the splitting assumes the form $\Delta m_\pi^2 = 2c_2a^2$, making it explicit that the splitting is an $O(a^2)$ effect. However, in the following we prefer to keep the notation as in (54).

The tree level result for the four degenerate kaon masses reads

$$m_K^2 = B(\mu_h + \delta + \mu_l) - \frac{8\rho^2}{f^2}W'_8. \quad (55)$$

Recall that the quark mass combinations on the right hand side correspond to the physical quark mass combination $(m_s + m)$. Thus the quark mass dependent part reproduces the known continuum ChPT expression.

Finally, the eta mass is related to the kaon and pion mass by the Gell-Mann-Okubo relation,

$$m_\eta^2 = \frac{1}{3}(4m_K^2 - m_{\pi^\pm}^2). \quad (56)$$

However, this relation holds only if the twist angles are equal in both the heavy and light sector. If that is not the case an additional $O(a^2)$ contribution proportional to $(\cos\omega_h - \cos\omega_l)^2$ appears on the right hand side [31].

The tree level masses we have derived enter the propagators that appear in our one-loop calculation. The only difference to the propagators in continuum ChPT [14] is the mass splitting between the charged and neutral pions, and one has to keep track of the flavor indices for the pions in loop diagrams.

The relevant vertices are obtained by expanding (52) to four powers in the pseudo scalar fields. Expressed in terms of the tree level masses (53) and (55) the vertices stemming from \mathcal{L}_2 are the vertices known from continuum ChPT. Additional vertices stem from \mathcal{L}_{a^2} , and the $O(a^2)$ vertices read

$$\begin{aligned} \mathcal{L}_{a^2,4\pi} = & \frac{8}{3}\frac{\rho^2}{f^4}W'_{68}\pi_3^2\pi^2 + \frac{1}{2}\frac{\rho^2}{f^4}W'_{78}\pi_h'^4 \\ & + \frac{16}{3}\frac{\rho^2}{f^4}W'_7\pi_3^2\pi_8^2 + \frac{4}{\sqrt{3}}\frac{\rho^2}{f^4}W'_{78}\pi_3\pi_8\pi_h'^2, \end{aligned} \quad (57)$$

where we introduced the short hand notation $\pi^2 = \sum_{i=1}^8 \pi_i^2$ and $\pi_h'^2 = \pi_4^2 + \pi_5^2 - \pi_6^2 - \pi_7^2$. We emphasize that (57) is the result for maximal twist. For twist angles $\omega_{l,h} \neq \pi/2$ many more terms contribute [31].

Note that the LEC W'_{68} in (57) can be expressed in terms of the tree level pion mass splitting. Therefore, provided the mass splitting is known from data, the associated four-pion coupling does not involve an unknown LEC. This will play a crucial role later on.

All the vertices lead to tadpole diagrams that contribute to the various self energies of the pseudo scalars. These diagrams result in standard divergent scalar integrals, which are conveniently regularized by dimensional regularization. The counterterms necessary for the renormalization are supplied by the NLO Lagrangian $\mathcal{L}_{p^2a^2} + \mathcal{L}_{Ma^2} + \mathcal{L}_{a^4}$. For the 2-flavor theory this Lagrangian was derived in [9]. It is straightforward to repeat the derivation for the 4-flavor theory and subsequently perform the reduction to the 3-flavor theory. However, for our purpose here it is not necessary to derive the NLO Lagrangian completely. It is sufficient to derive enough independent terms that provide the required counterterms for the pseudo scalar masses, and we list these terms in appendix A.

C. One-loop results

In order to present our results it is useful to follow [14] and introduce

$$\mu_P = \frac{m_P^2}{32\pi^2 f^2} \log \frac{m_P^2}{\mu^2}, \quad P = \pi^\pm, \pi^0, K, \eta, \quad (58)$$

as a short hand notation for the chiral logs. Various combinations of GL coefficients [14] appear and we introduce $L_{46} = 2L_6 - L_4$ and $L_{58} = 2L_8 - L_5$. With these definitions the NLO results for the charged pion and the kaon mass read

$$M_{\pi^\pm}^2 = m_{\pi^\pm}^2 \left[1 + \mu_{\pi^0} - \frac{1}{3}\mu_\eta + 8\frac{m_{\pi^\pm}^2}{f^2} (L_{46} + L_{58}) + 16\frac{m_K^2}{f^2} L_{46} + C_1 \frac{\rho^2}{f^4} \right], \quad (59)$$

$$\begin{aligned} M_K^2 = m_K^2 & \left[1 + \frac{2}{3}\mu_\eta + 8\frac{m_{\pi^\pm}^2}{f^2} L_{46} + 8\frac{m_K^2}{f^2} (2L_{46} + L_{58}) \right] \\ & - \frac{1}{2}\Delta m_\pi^2 \mu_{\pi^0} + \frac{8\rho^2}{f^2} W'_{78} \mu_K + C_2 \frac{\rho^2 m_{\pi^\pm}^2}{f^4} + C_3 \frac{\rho^2 m_K^2}{f^4} + C_4 \frac{\rho^4}{f^6}. \end{aligned} \quad (60)$$

Here the coefficients C_i are (combinations of) LECs in the NLO Lagrangian. We introduced appropriate inverse powers of f such that these coefficients are dimensionless.⁹

A rather trivial check of our results is whether the correct continuum limit is reached. Indeed, for $\rho \rightarrow 0$ we have $m_{\pi^0} \rightarrow m_{\pi^\pm}$ and our results reproduce the corresponding ones of continuum ChPT. The charged pion mass has been computed in 2-flavor tmWChPT in [9], and (59) reproduces this result as well once the contributions from the kaon and the eta are dropped.

Result (60) for the kaon mass is a new result of our charmless 3-flavor theory, so let us discuss it in more detail. The first line in (60) is exactly the continuum ChPT result of Gasser and Leutwyler. The second line contains the corrections due to the nonzero lattice spacing. The analytic corrections are more or less expected. For example, away from the continuum limit one expects the GL coefficients to depend on the lattice spacing. Expanding $L_{ij}(\rho^2) = L_{ij}(\rho^2 = 0) + \Delta_{ij}\rho^2$ the analytic terms in the continuum part generate the contributions proportional to C_2, C_3 . The new additional chiral logs involving the neutral

⁹ In that respect our convention differs from the one in Ref. [9] where dimensionful C_i 's were introduced.

pion and the kaon cannot be guessed from the continuum result which contains an eta chiral log only. The new chiral logs stem entirely from the two vertices in the first line of (57).

For the neutral pion mass we find to NLO the expression

$$M_{\pi^0}^2 = m_{\pi^\pm}^2 \left[1 + 2\mu_{\pi^\pm} - \mu_{\pi^0} - \frac{1}{3}\mu_\eta + 8\frac{m_{\pi^\pm}^2}{f^2} (L_{46} + L_{58}) + 16\frac{m_K^2}{f^2} L_{46} + \tilde{C}_1 \frac{\rho^2}{f^4} \right] + \Delta m_\pi^2 \left[1 - 4\mu_{\pi^0} - 2\mu_K - \frac{2}{3}\mu_\eta + \tilde{C}_2 \frac{m_K^2}{f^2} + \tilde{C}_3 \frac{\rho^2}{f^4} \right] + \frac{64}{3} \frac{\rho^2}{f^2} W_7' \mu_\eta. \quad (61)$$

The coefficients \tilde{C}_i are NLO LECs different from the ones in (59) and (60). Also this result converges to the correct continuum limit, and it reproduces the result in the 2-flavor theory if we drop all the contributions associated with the kaon and the eta. Taking the difference $M_{\pi^0}^2 - M_{\pi^\pm}^2$ we obtain the pion mass splitting to NLO. It has a rather complicated mass dependence involving all possible chiral logs.

D. Finite volume corrections and a first numerical test

In deriving our results we assumed an infinite space-time volume. Corrections due to a finite spatial volume [32] can be easily included. The FV corrections essentially amount to a simple replacement of the chiral logarithms, $\mu_P \rightarrow \mu_P + \delta_{\text{FV},P}$. Following the notation of Ref. [33] the FV correction is given by

$$\delta_{\text{FV},P} = \frac{m_P^2}{32\pi^2 f^2} \tilde{g}_1(m_P L), \quad (62)$$

with \tilde{g}_1 containing a sum over modified Bessel functions. The function \tilde{g}_1 drops off exponentially for large arguments, so we may expect the dominant source for FV corrections in the kaon mass to be given by the neutral pion contribution. Note that our result makes a definite prediction for these FV corrections provided the pion mass splitting is known.

The ETM collaboration has generated lattice data for two different volumes keeping the other parameters fixed [24]. These data can be used for a first test of our results. For convenience we have summarized the relevant data in table I. On the two lattices the central values for the kaon mass differ by 0.8%. The statistical errors are about 0.1% and 0.16%, respectively, so a FV effect is noticeable in the kaon mass.

The charged pion mass is about 310 MeV on both lattices, while the neutral pion is significantly lighter with $M_{\pi^0}/M_{\pi^\pm} \approx 0.48$ and 0.57, respectively. So the data is in the LCE regime and our results of the last subsection are applicable. With our result (60) the relative shift of the kaon mass caused by the neutral pion log, $\epsilon_{r,\pi^0} = |M_K(L_1) - M_K(L_2)|/M_K(L_2)$ reads

$$\epsilon_{r,\pi^0} = \frac{1}{128\pi^2 m_K^2 f^2} \left(\Delta m_\pi^2 m_{\pi^0}^2 \tilde{g}_1(m_{\pi^0} L) \Big|_{L=L_1} - \Delta m_\pi^2 m_{\pi^0}^2 \tilde{g}_1(m_{\pi^0} L) \Big|_{L=L_2} \right). \quad (63)$$

In principle the quantities Δm_π^2 and $m_{\pi^0}^2$ are independent of the volume and could be taken out of the difference on the right hand side. In practice, however, we use the measured

Ensemble	aM_{π^\pm}	aM_{π^0}	aM_K	af_π	L/a
A40.32	0.1415(04)	0.0811(50)	0.25666(23)	0.04802(13)	32
A40.24	0.1445(06)	0.0694(65)	0.25884(43)	0.04644(25)	24

TABLE I: Data for pseudo scalar masses and the pion decay constant taken from Refs. [4, 24]. The data for the decay constant is divided by $\sqrt{2}$ in order to account for the different normalization used in [24] for the decay constant. The data was generated with $\beta = 1.9$ corresponding to a lattice spacing $a \approx 0.09\text{fm}$. More details can be found in [24].

values for the pseudo scalar masses and the decay constant. The difference is of higher order in the chiral power counting. Still, the data for the neutral pion mass differs noticeably on the two lattices, although the significance of this difference is questionable in view of the large statistical error. We choose to take the measured central values for the two neutral pion masses and compute ϵ_r following (63). The result for this procedure reads

$$\epsilon_{r,\pi^0} \approx 0.0024(7) \quad (64)$$

The error in this estimate is completely dominated by the error for the neutral pion mass. The estimate (64) falls short by a factor 3 in explaining the observed FV effect. Nevertheless, it has the correct order of magnitude. In contrast, the FV shift due to the eta leads to a shift $\epsilon_{r,\eta} \approx 5 \cdot 10^{-5}$.¹⁰ This is about 50 times smaller than the π^0 contribution and cannot explain the measured FV effect. Note that the eta contribution is the only one in both continuum ChPT and in WChPT in the GSM regime. So the observed large FV shift in the kaon data supports our assumption that the data is indeed in the LCE regime. However, more data at various volumes and with different pion mass splittings is needed to corroborate this conclusion.

V. CONCLUDING REMARKS

Current twisted mass lattice QCD simulations show a sizable pion mass splitting due to explicit flavor symmetry breaking. Twisted mass WChPT provides formulae which can be used to assess the impact of a large pion mass splitting on the chiral extrapolation and on FV corrections caused by small neutral pion masses. In the case of 2-flavor WChPT such formulae were derived already some time ago.

The extension to 3-flavor WChPT turned out to be non-trivial. The reason is the charm quark that forms a twisted mass doublet together with the strange quark. This ties together strange and charm even if the charm quark is too heavy for the D mesons to be described by ChPT. In the first half of this paper we constructed a ‘charmless’ chiral Lagrangian based on a known 4-flavor Lagrangian that contains the charm quark degrees of freedom. We

¹⁰ The eta mass is given by (56). Alternatively it can be taken from Ref. [34] with no difference on our estimate.

essentially reverted the expansion in the charm quark mass and reabsorbed its effects in the LECs of the chiral theory. This procedure seems to be - at least to us - the most direct way to derive the appropriate chiral Lagrangian for $N_f = 2+1+1$ tm lattice QCD. A comparison with known results in the 4-flavor theory shows that we do reproduce the physics due to the light degrees of freedom.

Based on our chiral Lagrangian we computed the pseudo Goldstone boson masses to NLO in the LCE regime. As anticipated, additional chiral logs proportional to a^2 show up at this order, leading to a modified quark mass dependence. The final results contain quite a few additional LECs, and it remains to be seen if there are enough data to resolve all the additional terms in chiral fits.

The additional chiral logs imply additional FV corrections, in particular FV corrections from the neutral pion. Since this is by far the lightest pseudo scalar, these FV corrections are the dominant ones. The LECs entering this correction are directly related to the pion mass splitting. Therefore, these FV corrections are a parameter free prediction of our results if the mass splitting is known. A first comparison with numerical data showed that these FV corrections are in the ballpark, but still too small to account for the observed FV effects in the kaon mass.

The kaon mass is peculiar insofar that the continuum ChPT result to one loop contains an eta chiral log only. Since the eta is fairly heavy the associated FV corrections are tiny and way too small to explain the observed FV effects. Without the FV corrections due to the π^0 , which explain the data at least qualitatively, the large observed FV effect in M_K is hard to understand.

A natural next step is the computation of the decay constants in the charmless 3-flavor theory. It requires the charmless expression for the physical axial vector currents, which can be constructed following the steps we used for the construction of the charmless effective Lagrangian [35]. We expect modifications of the chiral formulae analogous to the ones we found for the masses, in particular larger FV corrections caused by neutral pion logs.

We finally remark that the charmless 3-flavor Lagrangian derived here is also the first step to describe the mixed action simulations of the ETM collaboration. In order to avoid an unwanted mixing in the heavy sector, simulations with Osterwalder-Seiler valence quarks are performed. The corresponding mixed action ChPT [36, 37] takes into account the different discretization effects in the valence and sea sector. The chiral Lagrangian for the latter is the one we have derived here.

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Appendix A: NLO terms for the LCE regime

The full NLO Lagrangian in the LCE regime of SU(2) WChPT was derived in Ref. [29]. For the SU(4) theory there exist more terms because Cayley-Hamilton relations for the group SU(2) were used in [29] that do not hold for SU(4). Writing down these additional terms would be a straightforward task. However, we refrain from giving them because for the present paper and most other applications the complete list of terms is not necessary. Here we simply need enough counterterms for the pseudo scalar masses, and for these the terms in [29] are sufficient. These terms read

$$\begin{aligned}
\mathcal{L}_{p^2 a^2}^{\text{SU}(4)} &= a_1 \rho^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle + a_2 \rho^2 \langle \partial_\mu \Sigma + \partial_\mu \Sigma^\dagger \rangle \langle \partial_\mu \Sigma + \partial_\mu \Sigma^\dagger \rangle \\
&\quad + a_3 \rho^2 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle + a_4 \rho^2 \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle \\
\mathcal{L}_{Ma^2}^{\text{SU}(4)} &= b_1 \rho^2 \langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \rangle + b_2 \rho^2 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle \langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \rangle \\
&\quad + b_3 \rho^2 \langle \Sigma + \Sigma^\dagger \rangle^2 \langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \rangle \\
\mathcal{L}_{a^4}^{\text{SU}(4)} &= h_1 \rho^4 \langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \rangle^2 + h_2 \rho^4 \langle \Sigma + \Sigma^\dagger \rangle^2
\end{aligned}$$

Here the coefficients a_j, b_j, h_j are NLO LECs. The charm quark degrees of freedoms can now be removed in each of these terms as in the LO Lagrangian. This leads to the following list of terms for the charmless 3-flavor theory:

$$\begin{aligned}
\mathcal{L}_{p^2 a^2} &= a_1 \rho^2 \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle + a_2 \rho^2 \langle \partial_\mu \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \partial_\mu \Sigma_3^\dagger \rangle \langle \partial_\mu \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \partial_\mu \Sigma_3^\dagger \rangle \\
&\quad + a_3 \rho^2 \langle \Sigma_3 \tilde{\Sigma}_l \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle \\
&\quad - 2a_3 \rho^2 \langle P_s(\Sigma_3 + \Sigma_3^\dagger) \rangle \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle \\
&\quad + a_4 \rho^2 \langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \Sigma_3 \tilde{\Sigma}_l \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \rangle, \\
\mathcal{L}_{ma^2} &= b_1 \rho^2 \langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \rangle + b_2 \rho^2 \langle \Sigma_3 \tilde{\Sigma}_l \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle \langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \rangle \\
&\quad - 2b_2 \rho^2 \langle P_s(\Sigma_3 + \Sigma_3^\dagger) \rangle \langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \rangle \\
&\quad + b_3 \rho^2 \langle \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle^2 \langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \rangle, \\
\mathcal{L}_{a^4} &= h_1 \rho^4 \left[\langle \Sigma_3 \tilde{\Sigma}_l \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle - 2 \langle P_s(\Sigma_3 + \Sigma_3^\dagger) \rangle \right]^2 \\
&\quad + h_2 \rho^4 \langle \Sigma_3 \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_3^\dagger \rangle^2.
\end{aligned}$$

Expanding these terms to two powers in the pseudo scalar fields we obtain the necessary counterterms for our calculation. The LECs enter in various combinations in these counterterms. It is not necessary to record how the LECs enter these linear combinations, as long as there are sufficiently many LECs such that all linear combinations are independent.

And this is indeed the case.

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